1-bromo,2,3,4,6,8,9-hexachloro-dibenzo-dioxin

Inchi: InChI=1S/C12HBrCl6O2/c13-4-6(17)7(18)8(19)12-10(4)21-11-5(16)2(14)1-3(15)9(11)20-
InchiKey: WDKXQHLCDSRHQV-UHFFFAOYSA-N
Formula: C12HBrCl6O2
SMILES: Clc1cc(Cl)c2c(c1Cl)Oc1c(Br)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 469.76

Physical Properties

Property code	Value	Unit	Source
gf	39.37	kJ/mol	Joback Method
hf	-153.99	kJ/mol	Joback Method
hfus	57.01	kJ/mol	Joback Method
hvap	94.63	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	8.268		Crippen Method
mcvol	224.240	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	923.92	K	Joback Method
tc	1203.14	K	Joback Method
tf	708.68	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.87	J/mol×K	923.92	Joback Method
cpg	461.87	J/mol×K	1156.61	Joback Method
cpg	456.10	J/mol×K	1110.07	Joback Method
cpg	450.53	J/mol×K	1063.53	Joback Method
cpg	445.05	J/mol×K	1016.99	Joback Method
cpg	439.53	J/mol×K	970.46	Joback Method
cpg	467.95	J/mol×K	1203.14	Joback Method
dvisc	0.0003272	Pa×s	923.92	Joback Method

dvisc	0.0003623	Pa×s	888.05	Joback Method
dvisc	0.0004046	Pa×s	852.17	Joback Method
dvisc	0.0004562	Pa×s	816.30	Joback Method
dvisc	0.0005202	Pa×s	780.43	Joback Method
dvisc	0.0006007	Pa×s	744.55	Joback Method
dvisc	0.0007039	Pa×s	708.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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